Covariant density functional theory: The role of the pion

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We investigate the role of the pion in Covariant Density Functional Theory. Starting from conventional Relativistic Mean Field (RMF) theory with a non-linear coupling of the σ-meson and without exchange terms we add pions with a pseudo-vector coupling to the nucleons in relativistic Hartree-Fock approximation. In order to take into account the change of the pion field in the nuclear medium the effective coupling constant of the pion is treated as a free parameter. It is found that the inclusion of the pion to this sort of density functionals does not destroy the overall description of the bulk properties by RMF. On the other hand, the non-central contribution of the pion (tensor coupling) does have effects on single particle energies and on binding energies of certain nuclei.

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Density functional theory plays an important role for the microscopic description of quantum mechanical many-body systems. Although this theory is in principle exact [1] if the exact energy functional is known, in nuclear physics one is far from being able to derive this functional from underlying QCD. At the moment all successful functionals in nuclear physics need phenomenological parameters. It is still one of the major goals of modern nuclear structure theory to find the optimal density functional. This will allow reliable predictions in areas presently not yet or possibly never accessible to experiments. This functional should be universal in the sense that the same functional with the same set of parameters is used all over the periodic table. In fact, by employing global effective interactions, adjusted to

properties of symmetric and asymmetric nuclear matter, and to bulk properties of few spherical nuclei, self-consistent mean-field models have achieved a high level of accuracy in the description of nuclear structure properties [2].

Relativistic versions of self-consistent mean field theories are based on the Walecka model [3]. In addition a density dependence has been introduced [4] through non-linear meson coupling and in open shell nuclei pairing correlations have been taken into account [5]. Two essential assumptions enter in these descriptions: exchange-terms and vacuum polarization are not included explicitly. This does not mean, however, that these important contributions are neglected. Together with correlation effects they are taken into account in a phenomenological way by the adjustment of the parameters to experimental data.

The relativistic Hartree approximation leads to a very good quantitative description of many nuclear properties, in particular those of the bulk, such as binding energies, radii, deformation parameters, giant resonances etc. The complicated structure of effective two- and many-body forces and correlations of all sorts are taken into account in a Lorentz invariant way by effective meson fields, classified by their quantum numbers spin J, parity P and isospin T, as for instance the σ-meson ($J^\pi = 0^+, T = 0$), the ω-meson ($J^\pi = 1^-, T = 0$), the ρ-meson ($J^\pi = 1^-, T = 1$), and possibly the δ-meson ($J^\pi = 0^+, T = 1$). It turns out that all these mesons have a relatively heavy mass. In the limit of infinite mass it would be possible to take into account the Fock terms in a Hartree theory, using the Fierz-transformation [6], as it is done in non-relativistic Skyrme functionals [7] since many years. However, there is also the pion with a relatively small mass of $m_\pi = 138$ MeV. Certainly, it is the most important meson. It carries the quantum numbers ($J^\pi = 0^-, T = 1$) and is closely connected to the chiral properties of QCD. Because of its pseudo-scalar character it leads to a tensor force. In ab-initio calculations based on bare nucleon-nucleon forces [8] this part of the force gives the largest contribution to the nuclear binding energy. A detailed study of the nucleon-nucleon force [9] shows that indeed the σ-meson can be understood to a large extend, by the correlated two-pion exchange. In the nuclear medium, nonrelativistic and relativistic Brueckner calculations [10] as well as models based on chiral perturbation theory [11] explain the largest part of the attractive effective interaction at intermediate distances by the contributions of the pions [12]. The pion, because of its negative parity, does not contribute on the Hartree level. Its major effect comes from the second and higher order diagrams in the correlated two-pion exchange. In the phenomenological theory they

are taken into account effectively through the σ meson. On the tree level, however, the one-pion exchange leads to a Fock term, which is not included in the conventional relativistic energy density functionals based on the simple Walecka model [5]. Because of the small mass of the pion and because of the long range of the corresponding effective force it is not clear whether a Fierz transformation can be applied here.

In the past the pion has been included in several relativistic Hartree-Fock calculations, as for instance in Refs: [13, 14, 15, 16, 17, 18]. However, the resulting equations of motion are rather complicated. They were mostly solved for nuclear matter and only for a few spherical nuclei with doubly closed shells. The numerical complexity in these computer codes made it for a long time impossible to carry out a systematic fit to the experimental data of many nuclei. Only recently a new method to solve these complicated integro-differential equations in r-space was implemented by Long *et al.* and improved parameter sets have been determined [19, 20] based on density dependent meson-nucleon coupling constants.

In recent years the role of the pion in nuclei has gained renewed interest. Although, so far, there is no direct experimental evidence, to connect the pion with some observables, the tensor contribution of the one-pion exchange force leads to very characteristic properties of the single particle spectra in nuclei. It has been observed in shell model calculations for exotic nuclei [21] that characteristic shifts of effective single particle levels can be traced back to the tensor interaction. It is noted that these levels are essential to reproduce experimental data which have also been observed directly in recent experiments by the Argonne group [22]. It has been shown [21] that the tensor force between protons in an orbit with $j_{>} = l_{\pi} + \frac{1}{2}$ (spin parallel to the orbital angular momentum) and neutrons in an orbit with $j_{<} = l_{\nu} - \frac{1}{2}$ (spin anti-parallel to the orbital angular momentum) is strongly attractive or vice versa. On the other side it is strongly repulsive if the protons as well as the neutrons sit in orbits with both spins parallel (or anti-parallel) to the orbital angular momenta.

Apart from an early investigation in the seventies [23], in all the successful conventional mean field calculations the tensor force has been neglected. In most cases the parameters of those functionals are adjusted only to bulk properties of nuclei. The change of the single particle energies discussed above is not seen in such calculations and therefore new versions of mean field models have been proposed recently [24, 25, 26, 27, 28, 29, 30]. Most of these investigations are done with zero range tensor forces and in several of them it is suggested that tensor forces have an influence on certain single particle states around the

magic numbers and that the inclusion of the tensor force is able to improve the mean field description and to reduce to some extent the observed deviation of theoretical single particle levels from their experimentally measured values [22].

The motivation of the present work is to investigate the role of the pion in RMF calculations and to give answers to questions such as, (a) is the inclusion of the pion really necessary for an improved description of data in finite nuclei, (b) what is the role of the non central part (tensor part) of one pion exchange interaction to the evolution of nuclear shell effects, and (c) is it necessary to include in the density functional a tensor force for future improved density functional theories. Having this in mind we decided to extend the present covariant density functional and to include the pion on the level of relativistic Hartree-Fock (RHF) theory.

In contrast to the investigations of Ref. [19, 20] we start from the conventional form of the energy density functional $E_{RMF}[\hat{\rho},\phi]$ with non-linear σ-couplings, but no exchange terms for the mesons $\phi_m = \sigma, \omega, \rho, A$. However, we add the Fock term $E_\pi[\hat{\rho}]$ representing the pseudo-vector pion propagator of Yukawa form:

$$E[\hat{\rho},\phi] = E_{RMF}[\hat{\rho},\phi] + E_\pi[\hat{\rho}] \tag{1}$$

As discussed above, exchange terms of the heavy σ, ω and ρ mesons are taken into account in this model in a phenomenological way by adjusting the parameters of the direct terms. Certainly this is not the case for the pion with its small mass. Obviously, this procedure to approximate the exchange terms for the other mesons by readjusted direct terms is a relatively economic approximation. It facilitates greatly the numerical calculations for the fitting procedure and, of course, enables the study of the net effect of the pion, as everything else is left unchanged. The total number of the parameters remains small and this to a large extent speeds up the fitting procedure, which is obviously now considerably more complicated due to the Fock term.

In this work the mass of the pion was fixed to its experimental mass $m_\pi = 138.0$ MeV. On the other hand the pion coupling constant, is treated as a free parameter which varies from its experimental value for free pions f_π to zero. In other words it was considered as an effective parameter by introducing the factor λ, with which the f_π value is multiplied.

Since the addition of the exchange terms representing the pion changes the energy functional considerably, we have to carry out a new fit for all the parameters entering this

TABLE I: The parameter sets obtained after a fit with fixed value or the pion-coupling constant $f_\pi^2 = \lambda f_\pi^{2(free)}$, for various values of the parameter λ.

	RHF(1.0)	RHF(1.5)	RH
M (MeV)	939.000	939.000	939.000
m_π (MeV)	138.000	138.000	138.000
g_ω	13.677	13.588	12.899
g_ρ	3.606	4.222	4.589
m_σ (MeV)	511.741	511.272	505.967
m_ω (MeV)	782.501	782.501	782.238
m_ρ (MeV)	763.000	763.000	763.000
g_σ	10.442	10.532	10.189
g_2 (fm^{-1})	-7.192	-8.417	-10.209
g_3	-23.248	-26.468	-28.612
λ	1.00	0.50	0.00
χ^2	310.00	168.00	75.00

functional. We adopted in the present study the philosophy and the procedure used for the derivation of the well known parameter set NL3 [31] excluding the nucleus ^{58}Ni. We took several fixed value for λ (between 0 and 1) and we performed fits for the remaining six parameters of the model, i.e. for the mass m_σ of the σ-meson, the coupling constants g_σ, g_ω, g_ρ and the two parameters g_2 and g_3 for the non-linear coupling of the σ-meson. In table 1 some representative results are shown. The RHF(1.0) set corresponds to a fit where the full free pion coupling constant is used ($\lambda = 1$). Parameter set RHF(0.5) is the one in which

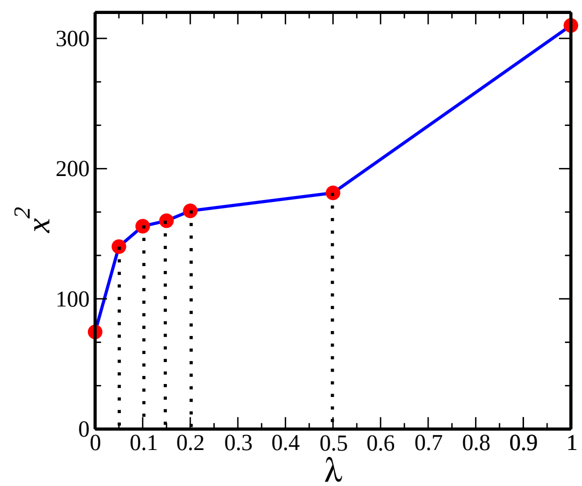

FIG. 1: (Color online) χ^2 of the fit as function of pion coupling constant in terms of the free pion coupling constant: λ is defined by $f_\pi^2 = \lambda f_\pi^{2(free)}$

tensor interaction induced by the pion is reduced by 50% as compared to its free value. Finally the RH set corresponds to a fit with $\lambda = 0$. In each case the χ^2 of the fit is calculated. The results shown in Fig. 1 indicate that the model, in its present form, does not favor the inclusion of the pion. This becomes clear from the χ^2 values which reflect the quality of the fit. In going from $\lambda = 1$ to $\lambda = 0$, i.e as the effect of the pion is reduced, the quality of the fit gradually improves. We investigated several isotopic chains of spherical nuclei using the various parameter sets. As expected, the bulk properties are not described so well in the case of finite values of λ. Of course, one does not observe any marked difference or peculiar behavior to these properties due to the presence of the pion. It is interesting, however, to investigate the influence on a microscopic level. For this purpose we studied two cases: 1) The variation of the single particle energies of certain levels in nuclei with magic numbers Z (or N) = 20 and Z (or N) = 28, and 2) the variation of the energy difference between the $1h_{11/2}$ and $1g_{9/2}$ single particle levels in Sn isotopes.

In Figs. 2 and 3 we show the variation of the single particle energies of the doublet $1f_{5/2}, 1f_{7/2}$ for neutrons, when we go along the corners of the rectangular in the (N,Z)-plane. We start with the doubly magic nucleus ^{40}Ca and add eight neutrons in the $\nu 1f_{7/2}$ shell. Let us first consider $\lambda = 0$, i.e. relativistic Hartree (RH) without pions. Here we observe relatively small shift in the single particle energies of the neutrons, because the increasing binding caused by the balance between σ and ω-fields is largely canceled by the ρ-field, which is repulsive for the neutrons. For the protons (Fig. 3) the ρ-field is attractive and

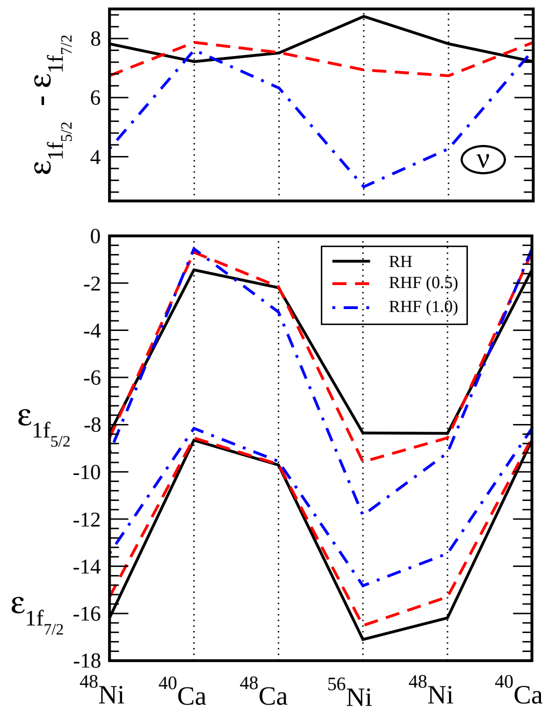

FIG. 2: (Color on line) The variation of the single particle energies (lower panel) and the spin orbit splitting (upper panel) of the doublet $1f_{7/2}, 1f_{5/2}$ for neutrons as one moves along the rectangular formed by the doubly magic nuclei ^{40}Ca, ^{48}Ca, ^{56}Ni, ^{48}Ni, ^{40}Ca.

therefore we find a strong lowering of the proton single particle energies when we go from ^{40}Ca to ^{48}Ca. Taking into account the Fock term caused by the pion tensor with a weight of 50 % (dashed lines in Figs. 2 and 3) or with a weight of 100 % (dashed-dotted lines) we find nearly no change for the neutron single particle levels, but a dramatic change for the proton single particle levels. The $\pi 1f_{7/2}$ is shifted upwards as compared to the pure Hartree calculation (full line), because, as we have seen the interaction between the neutrons in the $\nu 1f_{7/2}$ shell and the proton in the $\pi 1f_{7/2}$ shell is repulsive. On the other side the $\pi 1f_{5/2}$ orbit is shifted downward with respect to the pure Hartree calculation (full line), because the interaction between the neutrons in $\nu 1f_{7/2}$ shell and the proton in the $\pi 1f_{5/2}$ orbit is attractive. The changes follow the trends suggested in Ref. [21].

Next we start with the doubly magic nucleus ^{48}Ca and add eight protons in the $\pi 1f_{7/2}$ shell until we reach the nucleus ^{56}Ni. In this case we observe an analogous behavior. In relativistic Hartree (RH) without pions the proton levels change only slightly, because of the compensating effects of the ρ-field. However, the neutron levels are considerably shifted

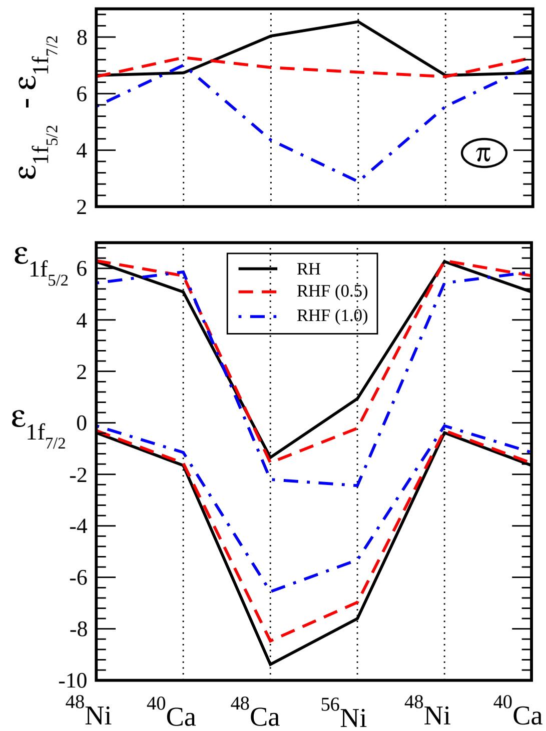

FIG. 3: (Color on line) The variation of the single particle energies (lower panel) and the spin orbit splitting (upper panel) of the doublet $1f_{7/2}, 1f_{5/2}$ for protons as one moves along the rectangular formed by the doubly magic nuclei ^{40}Ca, ^{48}Ca, ^{56}Ni, ^{48}Ni, ^{40}Ca.

downwards. Including the tensor field of the pions we observe again a repulsion for neutrons in the $\nu 1f_{7/2}$ shell and an attraction for the neutrons in the $\nu 1f_{5/2}$ shell, because in the first case both protons and neutrons have the configuration $j_>$, whereas in the second case the neutron $j_<$ and the proton has $j_>$, as it was predicted in Ref. [21].

Recently the energy difference between $\pi 1h_{11/2}$ and the $\pi 1g_{7/2}$ proton orbits in Sb-isotopes has been measured by the Sn(α, t) reaction [22] as a function of the neutron excess and it has been found that this difference increases steadily with the filling of the $\nu 1h_{11/2}$-orbit. This has been attributed to the tensor interaction in Refs. [21, 25], because this interaction is repulsive between the neutrons in the $\nu 1h_{11/2}$-orbit $(j_>)$ and the protons in the $\pi 1h_{11/2}$-orbit $(j_>)$ whereas it is attractive between the neutrons in the $\nu 1h_{11/2}$-orbit $(j_>)$ and the protons in the $\pi 1g_{7/2}$-orbit $(j_<)$. In Fig. 4 we show the variation of this energy difference $E_{1h_{11/2}} - E_{1g_{9/2}}$ on top of Sn isotopes as a function of the neutron number. The upper panel corresponds to the single particle levels of protons while the lower to those of neutrons. The s.p energies of Sn isotope with N=66 are taken as a reference point. In the case where the

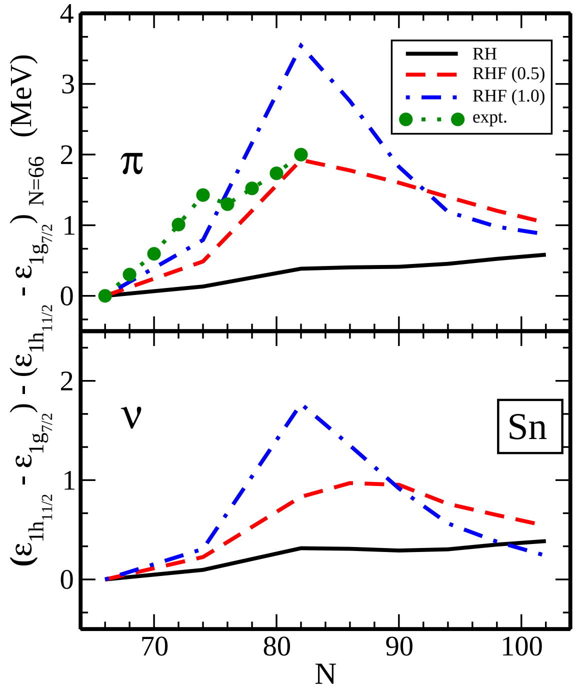

FIG. 4: (Color online) The evolution of the $1h_{11/2}$ and $2g_{9/2}$ neutron and proton energy gap. The s.p levels of ^{116}Sn are taken as reference point.

pion field is not taken into account (RH) this energy difference remains practically constant as the neutron number increases. The inclusion of the pion, however, changes the picture. As more neutrons are added the energy gap increases and from ^{116}Sn to ^{132}Sn the increase is of the order of 2-3 MeV. The effect grows steadily with the strength of the pion coupling and therefore it may be attributed to the tensor coupling in the pion nucleon interaction. The results for $\lambda = 0.5$ (RHF(0.5)) are in agreement with the experimental findings of Ref. [22]. As we see in the lower panel of Fig. 4 the effect seems to be less pronounced in the case of neutrons, as expected from the isospin dependence of the monopole part of the tensor force [21].

In Fig. 5 we study the influence of the tensor interaction on the binding energies B of doubly closed shell nuclei. We show the deviations $B_{th} - B_{exp}$ of theoretical results from experiment for various values of the strength parameter λ. Here we have to take into account that the binding energies of the nuclei ^{40}Ca, ^{48}Ca, ^{132}Sn, and ^{208}Pb have been used in the fit (see Table I of Ref. [31]). Therefore the deviations of the theoretical results from experimental data are all relatively small for these nuclei and we find big deviations only for the nucleus ^{100}Sn. The RMF-results without the pion produce an over-binding of 5.7

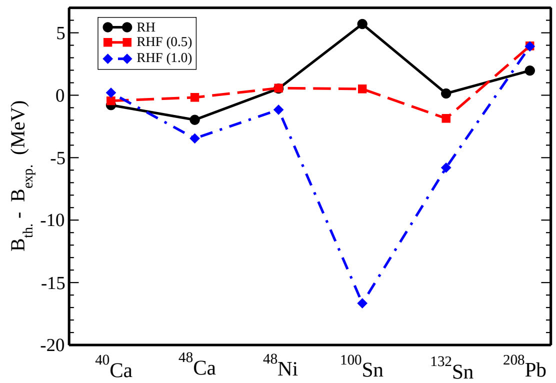

FIG. 5: (Color online) Differences between theoretical and experimental binding energies in doubly magic nuclei. RH calculations without the pion are compared with RHF calculations including the pion with the strength parameters $\lambda = 0.5$ and $\lambda = 1.0$.

MeV. The tensor force plays in the nucleus ^{100}Sn an important rule, because the $1g_{9/2}$-orbits ($j_>$) for protons and neutrons are both occupied by ten particles and the corresponding spin orbit partners $1g_{7/2}$-orbits ($j_<$) are empty. This force is repulsive and therefore we observe with increasing tensor force a reduced binding. For $\lambda = 0.5$ we are close to the experimental value.

In this work we have extended Covariant Density Functional Theory to include the pion degree of freedom on the Hartree-Fock level. This leads to tensor forces of finite range. In contrast to earlier investigations in Refs. [19, 20], where in the nuclear interior an exponentially decreasing pion-nucleon coupling was used, we have adjusted the parameters of the remaining non-linear RMF-Lagrangian for various coupling strengths of the pion field by extensive multi parameter χ^2 minimization procedures to reproduce bulk properties of infinite nuclear matter and spherical finite nuclei. The optimal fit is achieved for vanishing pion field. However, when considering the single particle levels in semi-magic nuclei, we observe, for finite pion fields, shifts in the particle levels in a consistent manner with the corresponding shell model calculations. It turned out that we can reproduce for roughly half the strength of the tensor force produced by the free pion the increasing energy difference between the $\pi 1h_{11/2}$ and the $\pi 1g_{7/2}$ orbits observed in recent Sn(α, t)-reactions in Argonne [22]. We also observe an influence of the tensor force on the binding energy in closed shell nuclei, where only one of the spin-orbits partners is occupied. Of course, so far, we stay on the mean field level, i.e. we do not consider coupling to low-lying surface phonons leading to an energy

dependent self energy and a fragmentation of the corresponding single particle energies [32]. Work in this direction is in progress.

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